Geostatistical Temporal/Spatial (GTS) Optimization Algorithm

X → **Identify Temporal Redundancy** → X1 → **Temporal Variogram Approach** ⇢ Preprocess Data & Construct Indicators (A)

Identify Temporal Redundancy ↓ X2 → **Iterative Thinning Approach** → Eliminate Wells with all NDs or with < 8-10 Observations

Preprocess Data & Construct Indicators (A) ↓ Compute Composite Temporal Variogram (B)

Eliminate Wells with all NDs or with < 8-10 Observations ↓ Estimate Slope & Confidence Bounds (D) → Initialize Thinning % Using C= 5% or 10%

Sampling intervals for eliminated wells can be adjusted using temporal variogram (X1)

Compute Composite Temporal Variogram (B) ↓ Determine Variogram Sill (C)

Initialize Thinning % Using C= 5% or 10% ↓ Perform Data Thinning → Re-compute Slope & Assess Accuracy (E)

Determine Variogram Sill (C) ↓ Adjust Global Sampling Frequency

Increase Thinning %

Perform Data Thinning

Re-compute Slope & Assess Accuracy (E) ↓

Slope still inbounds & Sign Unchanged?
- Y → Increase Thinning %
- N → Finalize Degree of Temporal Redundancy

Global sampling frequency should be applied to all wells except for those adjusted individually

Finalize Degree of Temporal Redundancy → Adjust Individual Well Sampling Frequencies

A

Preprocess Data & Construct Indicators

1. Examine Raw Dataset

Resolve data inconsistencies, fill in historical data gaps

Determine detection frequencies of each monitored parameter

Choose 1-3 critical monitoring parameters

2. Create Indicator Values

Exclude wells with no monitoring data or all NDs

Select parameters with highest detection rates or critical to remedial efforts

Choose indicator cutoff for each parameter

Convert concentrations to indicator values (IV)

Indicators: IV = 1 if concentration < cutoff; IV = 0 if concentration > cutoff

Cutoff can be quantitation limit, MCL, or site-specific regulatory limit

Compute minimum indicator across depths by well

Y

Wells screened at multiple depths?

N

Taking minimum indicator ensures value of 0 if concentration exceeds cutoff at any depth for given well

B

B

Compute Composite Temporal Variogram for Each Parameter

3. Compute Sample Variograms By Well

8-15 non-overlapping lags per spacing generally adequate

Pick two or three different lag spacings

Group data by well

Lags represent time intervals between sample dates

Group data pairs by lag separation

Infrequently sampled wells may only have few pairs per lag

Significant proportion of field/lab duplicates?

N

Y

Option: estimate variogram nugget using duplicates

Compute unidirectional variogram for each well & spacing

Weight this average by # lag pairs contributed by each well

Combine sample variograms w/ different lag spacings into a single variogram

4. Average variogram values across wells by lag

If lags from different spacings are identical, form weighted average of variogram values at that lag

C

C

5. Determine approximate variogram sill

Use a graphical non-linear smoother to help identify sill

Sill evident at some time interval (tmin)?

N   Y

Sill equals smallest time interval (lag) where variogram first plateaus or reaches highest point

Option: Try re-computing variogram with different lag spacing and/or different # lags

Individual well sampling frequencies may still be adjusted using (X2)

Do not use temporal variogram as basis for global minimum sampling interval

N   Sill now evident?   Y

Designate tmin as minimal sampling interval

Samples should be collected on an interval no shorter than tmin

Take largest tmin as minimum global sampling interval

Compare tmin values estimated for critical parameters

6. Adjust Global Sampling Frequency

Finalize sampling schedule & determine cost savings

All wells may be adjusted except for other superceding hydrogeologic or treatment considerations

Sampling interval can be longer than tmin, especially if indicated by individual well adjustment (X2)

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  D  ──────▶  Adjust Individual Well      ──────▶  1. Estimate        ──────▶  Plot time
              Frequencies for Each                 Linear Slope                series graph
              Critical Parameter                   via Sen's                   of well
                                                   Method                      concentrations
```

Typically need minimum of 8-10 measurements per well

Minimums: at least 2 most recent yrs of quarterly data or at least 8 distinct quarterly measurements

Set pairwise slope for any two NDs to 0

Construct sorted list of pairwise slopes for each distinct pair of sampling events or periods

80% to 90% confidence bounds should be adequate

Confidence bounds will equal particular pairwise slopes in the sorted list

Estimate confidence interval around slope estimate

Determine Sen's estimate as median pairwise slope value

2. Iteratively "thin" the data series

Initialize thinning % at C=5% or 10%

Sort dataset by sample date

Generate list of uniform random variates

D1

This weights data more equally across entire sampling record

Replace exact sampling date with midpoint of time period

Group sampling events into smaller set of equal-length time periods

"Remove" 1 of every successive group of (1/C) values in list

No pairwise slopes computed for events falling in same time period

Y

N

Highly irregular or "bunched" sampling?

Use lowest random variate in each group to tag values for removal

Recompute Sen's slope estimate on remaining values

E

E

3. Assess
Accuracy

Compare
re-computed
slope to original
confidence
bounds

Increase
thinning %
(e.g., by
5-10%)

Y Sign of slope
unchanged?

Y Re-computed
slope within
bounds?

N

N

D1

Gives estimate
of average
sampling interval

Set previous
lower C as final
thinning %

Set
parameter-specific
maximum
sampling interval
to this value

Divide total
time interval
by #
remaining pts

4. Adjust well
sampling
frequency

If early sampling is
more intensive or
"bunched" than
recent sampling,
exclude early portion
of sampling record

Compare
maximum
interval for
each critical
parameter

Set final well-specific
sampling interval to
smallest of these
maximums

Y

Identify Spatial Redundancy

Preprocess Data & Construct Indicators (F)

Limit analysis to 1-3 critical parameters

At least 30-40 wells usually needed; if # wells too small, just adjust sampling frequencies at existing wells using (X)

Initialize Wgt Threshold to 0

Model Spatial Covariance (G)

Perform Indicator Kriging (I)

Use Kriging Variances & Site Maps to Assess Uncertainty (J)

Use Kriging Wtgs to Tag Redundant Wells (L)

Increase Wgt Threshold

Small Change in Global Variance & Interpolated Maps?

Y

N

All wells with global wgts < threshold can be potentially removed from subsequent sampling

Typical wgts will depend on # of wells being kriged at the site

Pick threshold to tag at least 10-20% of remaining wells

Finalize List of Spatially Redundant Wells

Permanent removal must be negotiated with regulators, based on relevant hydrogeologic criteria

Compute Cost Savings from Removing Redundant Wells

F

Preprocess Data & Construct Indicators

1. Examine Raw Dataset

Resolve data inconsistencies, fill in historical data gaps

Determine detection frequencies of each monitored parameter

Select parameters with highest detection rates or critical to remedial efforts

Choose 1-3 critical monitoring parameters

2. Create Indicator Values

Remove wells with no monitoring data

Choose indicator cutoff for each parameter

Convert concentrations to indicator values (IV)

Indicators: IV = 1 if concentration < cutoff; IV = 0 if concentration > cutoff

Cutoff can be quantitation limit, MCL, or site-specific regulatory limit

Wells screened at multiple depths?

Y

N

E.g., by quarterly or semi-annual periods

Only use most recent 4-8 time slices

Group sampling events into equal-length time "slices"

Compute minimum indicator across depths by well

Irregular sampling frequencies?

Y

N

Compute minimum indicator across sampling dates within each time slice by well

Taking minimum indicator ensures value of 0 if concentration exceeds cutoff at any depth for given well or given time slice

Designate each distinct sampling date as a "time slice"

Group data by common sampling dates

G

```
( G ) ----> ⟨ Model Spatial
              Covariance ⟩
```

E.g., Lags of 100 ft versus lags of 200 ft versus lags of 400 ft

8-15 non-overlapping lags per spacing generally adequate

3. Compute Sample Variograms by Parameter for Each Time Slice

Pick two or three different lag spacings

Group data pairs by lag separation

Most lags should have at least 10-20 pairs; if not, increase lag spacing

Significant proportion of field/lab duplicates?

N

Y

Option: estimate variogram nugget using duplicates

Compute omnidirectional variogram for each lag spacing

For equal-sized (i.e., overlapping) lags, compute wgted average of variogram values

Combine sample variograms with different lag spacings into single variogram

Use isotropic variogram (i.e., ignoring pair direction) to model the combined variogram

H

```
    ( H ) - - - →  ┌─────────────┐ - - →      ◇ Pattern ◇ ──Y──→      ⬡ Averaging of
                   │ 4. Compare  │           ◇ similar   ◇              variogram
                   │ Sample      │           ◇ across time ◇            values occurs at
                   │ Variograms  │            ◇ slices? ◇               overlapping (i.e.,
                   │ Across Time │                │                     equal) lags, one
                   │ Slices for  │                │ N                   per time slice
                   │ Each        │                │
                   │ Parameter   │                ↓
                   └─────────────┘
```

4. Compare Sample Variograms Across Time Slices for Each Parameter

Pattern similar across time slices?

Y

N

Averaging of variogram values occurs at overlapping (i.e., equal) lags, one per time slice

Build separate variogram model for each slice

Average variograms across time slices

5. Build Model Variogram(s) for Each Parameter

Standard models: spherical, gaussian, exponential, & power

Feed sample variograms into non-linear model fitter

Restrict fitting algorithm to standard geostatistical models

Allow up to 3 nested model structures plus nugget term

Use wgted least squares fitting criterion

Fit criterion based on number of data pairs/lag to minimize effect of outliers

I

I

Perform Kriging on Data from Each Time Slice

Map estimates are wgted linear combinations of known sample data

Need enough blocks to gain adequate spatial resolution of concentration pattern

Typically need minimum of 30 to 40 wells

6. Create Interpolated Site Map for Each Time Slice & Parameter

Divide site area into non-overlapping blocks

If # of wells too small, only adjust sampling frequencies of existing wells using (X)

m = 4 to 16 points per block usually adequate

Use search algorithm to locate nearby known samples

Discretize each block into m unsampled locations

Search algorithm used repeatedly at each discretized point in each block

When re-kriging, keep same covariance model and block arrangement

1 sample required; maximum of 16 samples per search generally OK

7. Perform simple indicator kriging (IK)

I1

Using time slice-averaged variogram model?

Y

Perform kriging on each slice with same time-averaged model

N

Compute block variance estimates

Compute block kriging estimates

Perform kriging on any given slice with slice-specific variogram model

J

Compute local kriging (i.e., interpolation) wgts

J

Assess Uncertainty for Each Critical Parameter

This step gives global uncertainty measure for a particular well configuration

8. Check Global Kriging Variance

Average local block kriging variances across site by time slice

Average mean kriging variances across time slices

Compare global variance to previous estimate

Significant increase for any parameter?

N

Y

Increase wgt threshold

Look for relative changes of at least 10-20%

Select previous lower threshold as final cutoff

L

Finalize list of redundant wells

All wells with global wgts < threshold can be potentially removed from subsequent sampling

K

K

9. Check Ratio of Local Kriging Variances

For each block, compute ratio of local kriging variances from successive thresholds

Large ratios signify substantial increases in the estimation (i.e., kriging) variance

All wells with global wgts < threshold can be potentially removed from subsequent sampling

Generate map of local ratios

Helps identify site areas where more spatial information has been lost

Finalize list of redundant wells

Many areas with high ratios for any parameter?

Y   N

Select previous lower threshold as final cutoff

Increase wgt cutoff threshold

Too much detail lost at current threshold for any parameter?

Y   N

10. Compare Estimated Site Maps

Compare kriged maps of site at successive thesholds

This is a subjective but often valuable comparison

L

L

Tag Spatially Redundant Wells

11. Compute Average Global Kriging Wgts for Each Parameter

Accumulate & sum local kriging wgts by well & time slice

Divide each well's sum by # of kriged blocks

Average wgts across time slices by well

Sort well IDs by average wgts

Spatially redundant wells should have small wgts

Low wgts signify wells contributing little to estimated site maps

12. Compare each well to wgt threshold

Multiple constituents?

N   Y

Compute separate global wgts for each constituent

Average wgts across constituents

I1

Remove tagged wells from further computations

Classify well as redundant

Global kriging wgt < threshold?

Y

N

Classify well as essential